Chapter 5

Constitutive Modelling

5.1 Introduction

Thus far we have established four conservation (or balance) equations, an entropy inequality and a number of kinematic relationships. The overall set of governing equations are collected in Table 5.1. The Eulerian form has a one more independent equation because the density must be determined, whereas in the Lagrangian form it is directly related to the prescribed initial[1] density ρ_0. Lecture 14

Physical Law	Eulerian Form	N	Lagrangian Form	n
Kinematics:	$\frac{D\boldsymbol{R}}{Dt} = \boldsymbol{V}$,	3,	$\frac{\partial \boldsymbol{r}}{\partial t} = \boldsymbol{v}$,	3;
Mass:	$\frac{D\rho}{Dt} + \rho\, \boldsymbol{\nabla}_{\boldsymbol{R}}\boldsymbol{\cdot}\boldsymbol{V} = 0$,	1,	$\rho_0 = \rho J$,	0;
Linear momentum:	$\rho\frac{D\boldsymbol{V}}{Dt} = \boldsymbol{\nabla}_{\boldsymbol{R}}\boldsymbol{\cdot}\mathsf{T} + \rho\boldsymbol{F}$,	3,	$\rho_0\frac{\partial \boldsymbol{v}}{\partial t} = \boldsymbol{\nabla}_{\boldsymbol{r}}\boldsymbol{\cdot}\mathsf{p} + \rho_0\boldsymbol{f}$,	3;
Angular momentum:	$\mathsf{T} = \mathsf{T}^T$,	3,	$\mathsf{s} = \mathsf{s}^T$,	3;
Energy:	$\rho\,\frac{D\Phi}{Dt} = \mathsf{T} : \mathsf{D} + \rho B - \boldsymbol{\nabla}_{\boldsymbol{R}}\boldsymbol{\cdot}\boldsymbol{Q}$,	1,	$\rho_0\frac{\partial\phi}{\partial t} = \mathsf{s} : \dot{\mathsf{e}} + \rho_0 b - \boldsymbol{\nabla}_{\boldsymbol{r}}\boldsymbol{\cdot}\boldsymbol{q}$,	1;
Entropy inequality:	$\rho\frac{D\eta}{Dt} \geq -\boldsymbol{\nabla}_{\boldsymbol{R}}\boldsymbol{\cdot}\,(\boldsymbol{Q}/\Theta) + \rho B/\Theta$,	0,	$\rho_0\frac{\partial\eta_0}{\partial t} \geq -\boldsymbol{\nabla}_{\boldsymbol{r}}\,(\boldsymbol{q}/\theta) + \rho_0 b/\theta$,	0.
Independent Equations:		11	10	

Table 5.1: The governing equations for continuum mechanics in Eulerian and Lagrangian form. N is the number of independent equations in Eulerian form and n is the number of independent equations in Lagrangian form.

Examining the equations reveals that they involve more unknown variables than equations, listed in Table 5.2. Once again the fact that the density in the Lagrangian formulation is prescribed means that there is one fewer unknown compared to the Eulerian formulation. Thus, in either formulation and additional eleven equations are required to close the system. These additional equations are known as **constitutive** equations and describe the nature of the continuum under consideration by characterising the responses: stress, internal energy, entropy and heat flux in terms of the observable variables: the kinematics of the body and its temperature.

[1]It is the fact that information about the reference (initial) state is known in the Lagrangian formulation that reduces the number of equations to be solved.

Variable	Eulerian	M	Lagrangian	m	Relationship
Position:	$\boldsymbol{R}$,	3,	$\boldsymbol{r}$,	3,	$\boldsymbol{R}(\boldsymbol{r}, t)$;
Velocity	$\boldsymbol{V}$,	3,	$\boldsymbol{v}$,	3,	$\boldsymbol{V}(\boldsymbol{R}(\boldsymbol{r}, t), t) = \boldsymbol{v}(\boldsymbol{r}, t)$;
Density:	ρ,	1,	ρ_0,	0,	$\rho_0 = \rho J$;
Stress:	T	9	s or p	9	$\mathsf{s} = J\mathsf{F}^{-1}\mathsf{T}\mathsf{F}^{-T}$ or $\mathsf{p} = J\mathsf{T}\mathsf{F}^{-T}$;
Body Force:	$\boldsymbol{F}$,	0,	$\boldsymbol{f}$,	0,	$\boldsymbol{F}(\boldsymbol{R}(\boldsymbol{r}, t), t) = \boldsymbol{f}(\boldsymbol{r}, t)$;
Internal Energy:	Φ,	1,	ϕ,	1,	$\Phi(\boldsymbol{R}(\boldsymbol{r}, t), t) = \phi(\boldsymbol{r}, t)$;
Heat flux:	$\boldsymbol{Q}$,	3,	$\boldsymbol{q}$,	3,	$\boldsymbol{q} = J\boldsymbol{Q}F^{-T}$;
Heat supply:	B,	0,	b,	0,	$B(\boldsymbol{R}(\boldsymbol{r}, t), t) = b(\boldsymbol{r}, t)$;
Entropy:	η,	1,	η_0,	1,	$\eta(\boldsymbol{R}(\boldsymbol{r}, t), t) = \eta_0(\boldsymbol{r}, t)$;
Temperature:	Θ,	1,	θ,	1,	$\Theta(\boldsymbol{R}(\boldsymbol{r}, t), t) = \theta(\boldsymbol{r}, t)$;
Independent Variables:		22		21	

Table 5.2: The variables of continuum mechanics in Eulerian and Lagrangian form. M is the number of independent variables in Eulerian form and m is the number of independent variables in Lagrangian form. If M or m is 0 then the variable is prescribed.

Formulation the constitutive equations appropriate to different materials is known as constitutive modelling and falls somewhere between an art and a science. One approach is to start from a molecular theory assuming simple (or complex) mechanical laws for the molecular behaviour and then to average over all possible configurations to obtain the macroscopic (continuum) behaviour. This approach is used in the kinetic theory of gases, the development of constitutive models for polymeric fluids and rubbers. An alternative approach is entirely phenomenological: plausible models are suggested that describe observed phenomena. We can also always invoke a linear approximation that will be valid under small deviations, but will not remain valid over all possible motions. In fact, it has proved impossible to construct constitutive models that are valid over all possible ranges of motion for a given material.

However we reach it, our constitutive model should not violate the laws of thermodynamics and should obey certain physically reasonable principles; of course, exactly what is reasonable is a matter of endless debate. The most common principles are as follows:

- The present state of the material is determined entirely by its past history up to the present time; and the most recent states are the most important[2].
- The interactions between material points decays with increasing distance, so that the material behaviour of a particular point is dominated by the local behaviour in space (and time from above).
- Initially **all** constitutive equations should have the same independent variables.
- The constitutive equations should be objective (material frame indifferent).

[2]Things that happened a very long time ago have an imperceptible effect on the material.

- The constitutive equations should be invariant under transformations of the Lagrangian coordinates that preserve intrinsic symmetries of the material.

5.2 Axiom of Objectivity

In general, the motion of an observer will affect the values of measured physical quantities. The underlying behaviour of material should not depend on the motion of the observer, so we wish to understand how the apparent material properties change due to observer motion. A quantity that is independent of the observer is said to be *objective* or *material frame indifferent*.

An inertial frame of reference is a frame in which Newton's laws apply and so the results derived in chapters 3 and 4 apply only in inertial frames. Non-inertial frames introduce fictitious forces into the governing equations due to frame acceleration, *e.g.* Coriolis or centripetal/centrifugal forces, which is precisely because the acceleration is not objective.

We shall neglect relativistic effects which means that spatial distances and the time intervals between events measured by all observers must remain the same. We suppose that one observer measures spatial position and time by the pair $(\boldsymbol{R}, t)$ and another by the pair $(\boldsymbol{R}^*, t^*)$. If the distances between points and time between events must remain the same for both observers then the most general possible transformation is

$$\boldsymbol{R}^*(t^*) = \mathsf{Q}(t)\boldsymbol{R}(t) + \boldsymbol{C}(t), \qquad t^* = t - a, \tag{5.1}$$

where $\mathsf{Q}(t)$ is an orthogonal matrix, $\boldsymbol{C}(t)$ is an arbitrary point in space (or translation vector) and a is a constant time shift, which means that the material derivatives D/Dt and D/Dt^* coincide.

For a vector to be objective then its length must not change under the observer transformation, *i.e.*

$$\boldsymbol{A}^*\boldsymbol{\cdot}\boldsymbol{A}^* = \boldsymbol{A}\boldsymbol{\cdot}\boldsymbol{A}.$$

Now if we define a vector to be the difference between to points in space, $\boldsymbol{A}(t) = \boldsymbol{R}(t) - \boldsymbol{S}(t)$, then

$$\boldsymbol{A}^*(t) = \boldsymbol{R}^*(t) - \boldsymbol{S}^*(t) = \mathsf{Q}(t)\boldsymbol{R}(t) + \boldsymbol{C}(t) - \mathsf{Q}(t)\boldsymbol{S}(t) - \boldsymbol{C}(t) = \mathsf{Q}(t)[\boldsymbol{R}(t) - \boldsymbol{S}(t)] = \mathsf{Q}\boldsymbol{A}.$$

Hence, writing out the components in Cartesian coordinates

$$\boldsymbol{A}^*\boldsymbol{\cdot}\boldsymbol{A}^* = A_I^*A_I^* = Q_{IJ}A_JQ_{IK}A_K = Q_{KI}^TQ_{IJ}A_JA_K = \delta_{KJ}A_JA_K = A_JA_J = \boldsymbol{A}\cdot\boldsymbol{A},$$

because Q is orthogonal. Thus the vector is objective if

$$\boldsymbol{A}^* = \mathsf{Q}\boldsymbol{A},$$

which is equivalent to saying that the vector satisfies the appropriate tensor transformation laws in order to remain invariant under the observer transformation. Hence, for a tensor of order two, M, to remain invariant under observer transformation it must obey the transformation rule

$$\mathsf{M}^* = \mathsf{Q}\mathsf{M}\mathsf{Q}^T.$$

For higher order tensors, the appropriate transformation rules will apply.

5.2.1 Non-objectivity of velocity and acceleration

Taking the material derivative of equation (5.1), and suppressing the explicit dependence on time, gives the transformations for the velocity and acceleration

$$\boldsymbol{V}^* = \frac{D\boldsymbol{R}^*}{Dt^*} = \frac{D}{Dt}\left(\mathsf{Q}\boldsymbol{R} + \boldsymbol{C}\right) = \dot{\mathsf{Q}}\boldsymbol{R} + \mathsf{Q}\dot{\boldsymbol{R}} + \dot{\boldsymbol{C}} = \mathsf{Q}\boldsymbol{V} + \dot{\mathsf{Q}}\boldsymbol{R} + \dot{\boldsymbol{C}}, \tag{5.2a}$$

and

$$\boldsymbol{A}^* = \frac{D\boldsymbol{V}^*}{Dt^*} = \mathsf{Q}\boldsymbol{A} + 2\dot{\mathsf{Q}}\boldsymbol{V} + \ddot{\mathsf{Q}}\boldsymbol{R} + \ddot{\boldsymbol{C}}, \tag{5.2b}$$

where the overdot indicates the material derivative. Hence, as we already know, the velocity and acceleration are not objective and depend on the motion of the observer.

We can give physical interpretation to the non-objective terms in equation (5.2a,b) by introducing the observer spin tensor, $\Omega = \dot{\mathsf{Q}}\mathsf{Q}^T$, associated with the observer transformation. Taking the material derivative of the identity $\mathsf{Q}\mathsf{Q}^T = \mathsf{I}$ gives

$$\dot{\mathsf{Q}}\mathsf{Q}^T + \mathsf{Q}\dot{\mathsf{Q}}^T = \Omega + \Omega^T = 0,$$

which shows that Ω is antisymmetric, so $\Omega = -(\dot{\mathsf{Q}}\mathsf{Q}^T)^T = -\mathsf{Q}\dot{\mathsf{Q}}^T$.

Inverting equation (5.1) we obtain $\boldsymbol{R} = \mathsf{Q}^T(\boldsymbol{R}^* - \boldsymbol{C})$, which can be used in equation (5.2a) to write

$$\boldsymbol{V}^* - \mathsf{Q}\boldsymbol{V} = \dot{\mathsf{Q}}\mathsf{Q}^T(\boldsymbol{R}^* - \boldsymbol{C}) + \dot{\boldsymbol{C}} = \dot{\boldsymbol{C}} + \Omega(\boldsymbol{R}^* - \boldsymbol{C}).$$

If the terms on the right-hand side were zero, the velocity would be objective. The first term reflects the relative velocity of the observers and the second is their relative rotation[3]. Thus non-zero relative velocity or relative rotation between observers leads to the non-objective differences in velocity.

Inverting the relationship for velocity, we obtain $\boldsymbol{V} = \mathsf{Q}^T\left[V^* - \dot{\boldsymbol{C}} - \Omega(\boldsymbol{R}^* - \boldsymbol{C})\right]$ and using this and the inverse relationship for position in equation (5.2b) we obtain

$$\boldsymbol{A}^* - \mathsf{Q}\boldsymbol{A} = \ddot{\boldsymbol{C}} + 2\dot{\mathsf{Q}}\mathsf{Q}^T\left[\boldsymbol{V}^* - \dot{\boldsymbol{C}} - \Omega(\boldsymbol{R}^* - \boldsymbol{C})\right] + \ddot{\mathsf{Q}}\mathsf{Q}^T(\boldsymbol{R}^* - \boldsymbol{C}),$$

$$= \ddot{\boldsymbol{C}} + 2\Omega(\boldsymbol{V}^* - \dot{\boldsymbol{C}}) + (\dot{\Omega} - \Omega^2)(\boldsymbol{R}^* - \boldsymbol{C}),$$

after using the fact that $\dot{\Omega} = \ddot{\mathsf{Q}}\mathsf{Q}^T - \dot{\mathsf{Q}}\dot{\mathsf{Q}}^T = \ddot{\mathsf{Q}}\mathsf{Q}^T - \dot{\mathsf{Q}}\mathsf{Q}^T\mathsf{Q}\dot{\mathsf{Q}}^T = \ddot{\mathsf{Q}}\mathsf{Q}^T + \Omega^2$. The acceleration would be objective if the terms on the right-hand side were zero. The first term is the translational acceleration; the second is the Coriolis acceleration; the third combines the rotational and centripetal accelerations.

We conclude that the acceleration and velocity are only objective if the transformation is Galilean: $\boldsymbol{C}$ and Q are both constants, which means that the observers are not rotating or translating relative to each other.

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[3]The product of an antisymmetric tensor and a vector can be written as the cross product of two vectors:

$$\Omega_{IK}A_K = e_{IMK}\omega_M A_K \quad \Rightarrow \quad \Omega_{IK} = e_{IMK}\omega_M \quad \Rightarrow \quad e_{JKI}\Omega_{IK} = e_{JKI}\,e_{IMK}\,\omega_M,$$

$$\Rightarrow \quad e_{JKI}\Omega_{IK} = [\delta_{JM}\delta_{KK} - \delta_{JK}\delta_{MK}]\,\omega_M = 3\omega_J - \omega_J = 2\omega_J.$$

$$\Rightarrow \quad \omega_J = \frac{1}{2}e_{JKI}\Omega_{IK}.$$

If the two observers are not translating relative to one another $\boldsymbol{C} = \boldsymbol{0}$ then for a fixed vector $\boldsymbol{R}$, we can write

$$\frac{D\boldsymbol{R}^*}{Dt} = \Omega\boldsymbol{R}^* = \frac{1}{2}\boldsymbol{\omega} \times \boldsymbol{R}^*,$$

which expresses a rigid-body rotation about the axis $\boldsymbol{\omega}$ with angular velocity $|\boldsymbol{\omega}|/2$.

5.2.2 Objectivity of deformation measures

The deformation gradient tensor transforms via

$$F^*_{IJ} = \frac{\partial X^*_I}{\partial x_J} = \frac{\partial}{\partial x_J}\left\{Q_{IK}(t)X_K(t) + C_I(t)\right\} = Q_{IK}F_{KJ},$$

or

$$\mathsf{F}^* = \mathsf{Q}\,\mathsf{F},$$

so the deformation gradient tensor is not objective because it is a tensor of second order, but transforms like an objective vector[4]. The (right) Cauchy-Green tensor is invariant under change of observer because

$$\mathsf{c}^* = \mathsf{F}^{*T}\mathsf{F}^* = (\mathsf{QF})^T\mathsf{QF} = \mathsf{F}^T\mathsf{Q}^T\mathsf{QF} = \mathsf{F}^T\mathsf{F} = \mathsf{c};$$

and hence so is the Green–Lagrange strain tensor

$$\mathsf{e}^* = \frac{1}{2}\left(\mathsf{c}^* - \mathsf{I}^*\right) = \frac{1}{2}\left(\mathsf{c} - \mathsf{I}\right) = \mathsf{e}.$$

Thus, these tensors are not objective in the Eulerian sense described above because they are based on the Lagrangian, rather than the Eulerian, coordinates. Such quantities are sometimes called objective in a Lagrangian sense or observer invariant, rather than observer independent. The Eulerian (Almansi) strain tensor is based on the Eulerian coordinates and does transform objectively

$$\mathsf{E}^* = \frac{1}{2}\left(\mathsf{I}^* - \mathsf{C}^*\right) = \frac{1}{2}\left(\mathsf{QQ}^T - \mathsf{F}^{*-T}\mathsf{F}^{*-1}\right) = \frac{1}{2}\left(\mathsf{QQ}^T - \mathsf{QF}^{-T}\mathsf{F}^{-1}\mathsf{Q}^T\right) = \mathsf{QEQ}^T.$$

5.2.3 Objectivity of rate of deformation measures

The transformation of the Eulerian velocity gradient tensor, L, can be obtained by using the relationship (2.51)

$$\dot{\mathsf{F}} = \mathsf{LF} \quad\Rightarrow\quad \mathsf{L} = \dot{\mathsf{F}}\mathsf{F}^{-1};$$

and so

$$\mathsf{L}^* = \dot{\mathsf{F}}^*\mathsf{F}^{*-1} = \frac{D}{Dt}\left(\mathsf{QF}\right)\mathsf{F}^{-1}\mathsf{Q}^T = \left(\dot{\mathsf{Q}}\mathsf{F} + \mathsf{Q}\dot{\mathsf{F}}\right)\mathsf{F}^{-1}\mathsf{Q}^T = \mathsf{QLQ}^T + \dot{\mathsf{Q}}\mathsf{Q}^T = \mathsf{QLQ}^T + \Omega.$$

It follows that the symmetric part of the velocity gradient tensor, the Eulerian rate of deformation tensor transforms objectively

$$\mathsf{D}^* = \frac{1}{2}\left(\mathsf{L}^* + \mathsf{L}^{*T}\right) = \frac{1}{2}\left(\mathsf{QLQ}^T + \Omega + \mathsf{QL}^T\mathsf{Q}^T + \Omega^T\right) = \mathsf{Q}\frac{1}{2}\left(\mathsf{L} + \mathsf{L}^T\right)\mathsf{Q}^T = \mathsf{QDQ}^T, \qquad (5.3a)$$

but that the antisymmetric part, the spin tensor, does not

$$\mathsf{W}^* = \frac{1}{2}\left(\mathsf{L}^* - \mathsf{L}^{*T}\right) = \frac{1}{2}\left[\mathsf{Q}\left(\mathsf{L} - \mathsf{L}^T\right)\mathsf{Q}^T + \Omega - \Omega^T\right] = \mathsf{QWQ}^T + \Omega. \qquad (5.3b)$$

Naturally, this is completely consistent with our analysis of velocity and acceleration in §5.2.1, which showed that any measure involving relative rotation is non-objective. Equation (5.3b) reveals that the difference in instantaneous rotation rate measured by two different observers will differ by the relative rotation rate Ω. The equation can be written in the form

$$\mathsf{W} = \mathsf{Q}^T\left(\mathsf{W}^* - \Omega\right)\mathsf{Q},$$

which demonstrates that the spin tensor can be made objective by subtracting the non-inertial observer rotation rate Ω.

[4]The reason is because the deformation gradient tensor is two-point in character; the index associated with the Eulerian coordinate transforms objectively, but the index associated with the Lagrangian coordinate does not change under an Eulerian observer transformation.

5.2.4 Objective Rates

We have already seen that the material derivative of an objective quantity (a vector for example) is not objective because the velocity of the observer affects the perceived motion. If we work in Lagrangian framework the problem does not arise because the material derivative is objective in the Lagrangian sense, or observer invariant. Unfortunately, there are many circumstances in which we must work in the Eulerian framework, *e.g.* taking laboratory measurements or even applying boundary conditions. Thus, we are lead to consider rates of change that are objective in Eulerian formulations.

Vectors

The idea of objective rates is to construct derivatives that follow the motion in a more general sense than simple material derivatives, which follow the movement only of material points and therefore have no information about stretch or rotation of the continuum. Consider a vector field, $\boldsymbol{b}(\xi^i, t)$, that is convected with the motion of the continuum, so that it obeys the same transformation rules as line elements. In the undeformed configuration we have $\boldsymbol{b}(t = 0) = b^k(0)\boldsymbol{g}_k$ and then in the deformed configuration

$$\boldsymbol{B}(t) = B^{\overline{k}}\boldsymbol{G}_{\overline{k}}, \quad \text{where} \quad B^{\overline{k}}(t) = \frac{\partial \chi^{\overline{k}}}{\partial \xi^i}(t)\, b^i(t),$$

which follows from interpreting the motion as a coordinate transformation from Lagrangian ξ^i to Eulerian $\chi^{\overline{j}}$ coordinates and applying the standard contravariant transformation rule. Hence,

$$\boldsymbol{B}(t) = \frac{\partial \chi^{\overline{k}}}{\partial \xi^i}\, b^i\, \boldsymbol{G}_{\overline{k}} = \frac{\partial \chi^{\overline{k}}}{\partial \xi^i}\, b^i\, \frac{\partial \boldsymbol{R}}{\partial \chi^{\overline{k}}} = b^i\, \frac{\partial \boldsymbol{R}}{\partial \xi^i} = b^i \boldsymbol{G}_i = B^i \boldsymbol{G}_i,$$

so the convected vector is simply given by the components $B^i = b^i(t)$ in the base vectors associated with the Lagrangian coordinates in the deformed configuration, or convected base vectors.

Taking the material derivative of $\boldsymbol{B}$ gives

$$\frac{D\boldsymbol{B}}{Dt} = \frac{\partial B^k}{\partial t}\boldsymbol{G}_k + B^k \frac{D\boldsymbol{G}_k}{Dt} = \frac{\partial B^l}{\partial t}\boldsymbol{G}_l + B^k V^l||_k \boldsymbol{G}_l = \left[\frac{\partial B^l}{\partial t} + B^k V^l||_k\right]\boldsymbol{G}_l,$$

after using equation (2.46). The first term is a vector that will transform objectively because the material (partial) derivative of B^l (the Lagrangian coefficients) is invariant under observer transformation and the base vectors transform appropriately $\boldsymbol{G}_i^* = \mathsf{Q}\boldsymbol{G}_i$. The second term involves the covariant derivative with respect to the basis $\boldsymbol{G}_i$ or $\boldsymbol{G}_i^*$ depending on the observer. Hence it will not remain invariant under observer transformation and it is this term that renders the material derivative non objective. If we decompose the material derivative directly into components in the convected basis, $D\boldsymbol{B}/Dt = (DB^k/Dt)\,\boldsymbol{G}_k$, then we have that

$$\frac{DB^k}{Dt} = \frac{\partial B^k}{\partial t} + B^l V^k||_l.$$

The material and partial derivatives do not coincide in the convected basis because the convected base vectors change with time. Thus, an objective derivative can be formed by taking the vector

$$\boldsymbol{B}^{\nabla} = \frac{\partial B^k}{\partial t}\boldsymbol{G}_k = B^{\nabla k}\boldsymbol{G}_k, \quad \text{where} \quad B^{\nabla k} = \frac{DB^k}{Dt} - B^l V^k||_l.$$

The equation is a tensor equation so we can simply transform to the Eulerian coordinates $\chi^{\bar{i}}$ to obtain

$$B^{\nabla\bar{k}} = \frac{DB^{\bar{k}}}{Dt} - B^{\bar{l}}V^{\bar{k}}||_{\bar{l}} = \frac{\partial B^{\bar{k}}}{\partial t} + V^{\bar{i}}B^{\bar{k}}||_{\bar{i}} - B^{\bar{l}}V^{\bar{k}}||_{\bar{l}},$$

which can be written in vector form as

$$\boldsymbol{B}^{\nabla} = \frac{D\boldsymbol{B}}{Dt} - \mathsf{L}\boldsymbol{B},$$

and is called the upper convected (Oldroyd) derivative and represents a derivative that is taken following the motion of material lines. Note that if $\boldsymbol{B}^{\nabla} = \boldsymbol{0}$, the vector is invariant under the motion[5]. Note also that $\boldsymbol{V}^{\nabla} = \frac{\partial \boldsymbol{V}}{\partial t}$, because when the observer is moving with the material lines of the continuum the acceleration is due only to the acceleration of material particles, which is indeed independent of the observer.

The upper convected derivative can also be obtained by considering the material derivative of a vector and writing the vector as the product of the deformation gradient tensor and the undeformed vector in order to isolate an objective derivative

$$\frac{D\boldsymbol{B}}{Dt} = \frac{D}{Dt}\left(\mathsf{F}\boldsymbol{b}\right) = \frac{D\mathsf{F}}{Dt}\boldsymbol{b} + \mathsf{F}\frac{D\boldsymbol{b}}{Dt}.$$

The final term transforms objectively because the material derivative of a Lagrangian vector is invariant under observer transformation and the deformation gradient transforms as an objective vector $\mathsf{F}^* = \mathsf{QF}$. Thus, the objective upper convected derivative is obtained by

$$\boldsymbol{B}^{\nabla} = \frac{D\boldsymbol{B}}{Dt} - \frac{D\mathsf{F}}{Dt}\boldsymbol{b} = \frac{D\boldsymbol{B}}{Dt} - \frac{D\mathsf{F}}{Dt}\mathsf{F}^{-1}\boldsymbol{B} = \frac{D\boldsymbol{B}}{Dt} - \mathsf{LFF}^{-1}\boldsymbol{B} = \frac{D\boldsymbol{B}}{Dt} - \mathsf{L}\boldsymbol{B}.$$

This derivation does not reveal the provenance of the name upper convected, which arises because the derivative represents the material derivative of the upper (contravariant) components of a vector when convected with the motion. We confirm that the derivative is, in fact objective, from

$$\boldsymbol{B}^{*\nabla} = \frac{D\boldsymbol{B}^*}{Dt} - \mathsf{L}^*\boldsymbol{B}^* = \frac{D\mathsf{Q}\boldsymbol{B}}{Dt} - (\mathsf{QLQ}^T + \Omega)\mathsf{Q}\boldsymbol{B},$$

$$\Rightarrow \quad \boldsymbol{B}^{*\nabla} = \dot{\mathsf{Q}}\boldsymbol{B} + \mathsf{Q}\dot{\boldsymbol{B}} + \mathsf{QL}\boldsymbol{B} - \Omega\mathsf{Q}\boldsymbol{B} = \Omega\boldsymbol{Q}\boldsymbol{B} - \Omega\mathsf{Q}\boldsymbol{B} + \mathsf{Q}\left[\frac{D\boldsymbol{B}}{Dt} - \mathsf{L}\boldsymbol{B}\right] = \mathsf{Q}\boldsymbol{B}^{\nabla},$$

where the definition $\Omega = \dot{\mathsf{Q}}\mathsf{Q}^T$ has been used.

If we apply the same considerations to $\boldsymbol{B} = B_k\boldsymbol{G}^k$, then we would obtain the lower convected derivative

$$B^{\Delta}_{\bar{k}} = \frac{DB_{\bar{k}}}{Dt} + B_{\bar{l}}V^{\bar{l}}||_{\bar{k}} = \frac{\partial B_{\bar{k}}}{\partial t} + V^{\bar{i}}B_{\bar{k}}||_{\bar{i}} + B_{\bar{l}}V^{\bar{l}}||_{\bar{k}},$$

which can be written in vector form as

$$\boldsymbol{B}^{\Delta} = \frac{D\boldsymbol{B}}{Dt} + \mathsf{L}^T\boldsymbol{B}.$$

The lower convected derivative has not found to be as useful in describing the behaviour of continua as the upper convected derivative because it describes a derivative taken following material areas in

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[5]This is not entirely obvious, but can be easily derived because $\boldsymbol{B}^{\nabla} = 0$ implies that $\partial b^i/\partial t = 0$ and so the vector is invariant in the Lagrangian viewpoint and the transformation to Eulerian coordinates $B^{\bar{k}} = (\partial\chi^{\bar{k}}/\partial\xi^i)b^i$ ensures that $\boldsymbol{B}$ remains invariant.

an incompressible medium, or the product of material areas and a mass density in a compressible medium.

The upper and lower convective derivatives take the complete deformation into account, but we know that non-objectivity only arises through relative rotation of the observers. We can formulate the co-rotational or Jaumann rate by using the polar decomposition $\mathsf{F} = \mathsf{RU}$ to consider the material derivative of a vector that rotates, but does not stretch with the deformation

$$\frac{D\boldsymbol{B}}{Dt} = \frac{D}{Dt}(\mathsf{R}\boldsymbol{b}) = \frac{D\mathsf{R}}{Dt}\boldsymbol{b} + \mathsf{R}\frac{D\boldsymbol{b}}{Dt}.$$

As above, the second term transforms objectively because the rotation of the observer simply changes the rotation matrix[6] $\mathsf{R}^* = \mathsf{QR}$. Thus, we can form an objective derivative by taking

$$\overset{\circ}{\boldsymbol{B}} = \frac{D\boldsymbol{B}}{Dt} - \frac{D\mathsf{R}}{Dt}\boldsymbol{b}.$$

We can find the material derivative of the rotation tensor by considering using the polar decomposition

$$\frac{D\mathsf{F}}{Dt} = \frac{D\mathsf{R}}{Dt}\mathsf{U} + \mathsf{R}\frac{D\mathsf{U}}{Dt} = \mathsf{LF} = \mathsf{LRU},$$

so that

$$\mathsf{L} = \left(\frac{D\mathsf{R}}{Dt}\mathsf{U} + \mathsf{R}\frac{D\mathsf{U}}{Dt}\right)\mathsf{U}^{-1}\mathsf{R}^T = \dot{\mathsf{R}}\mathsf{R}^T + \mathsf{R}\dot{\mathsf{U}}\mathsf{U}^{-1}\mathsf{R}^T,$$

and hence

$$\mathsf{D} = \frac{1}{2}\left(L + L^T\right) = \frac{1}{2}\left(\dot{\mathsf{R}}\mathsf{R}^T + \mathsf{R}\dot{\mathsf{R}}^T\right) + \frac{1}{2}\mathsf{R}\left(\dot{\mathsf{U}}\mathsf{U}^{-1} + \mathsf{U}^{-1}\dot{\mathsf{U}}\right)\mathsf{R}^T,$$

but because R is orthogonal $D(\mathsf{R}^T\mathsf{R})/Dt = D\mathsf{I}/Dt = 0$ and so $\dot{\mathsf{R}}\mathsf{R}^T + \mathsf{R}\dot{\mathsf{R}}^T = 0$, which yields

$$\mathsf{D} = \frac{1}{2}\mathsf{R}\left(\dot{\mathsf{U}}\mathsf{U}^{-1} + \mathsf{U}^{-1}\dot{\mathsf{U}}\right)\mathsf{R}^T \quad \text{and} \quad \mathsf{W} = \frac{1}{2}\left(L - L^T\right) = \dot{\mathsf{R}}\mathsf{R}^T + \frac{1}{2}\mathsf{R}\left(\dot{\mathsf{U}}\mathsf{U}^{-1} - \mathsf{U}^{-1}\dot{\mathsf{U}}\right)\mathsf{R}^T.$$

If we neglect the deformation of the motion then $\dot{\mathsf{U}} = 0$, and $\mathsf{W} = \dot{\mathsf{R}}\mathsf{R}^T$, which means that $\dot{\mathsf{R}} = \mathsf{WR}$. Finally,we obtain the standard expression for the Jaumann rate

$$\overset{\circ}{\boldsymbol{B}} = \frac{D\boldsymbol{B}}{Dt} - \mathsf{WR}\boldsymbol{b} = \frac{D\boldsymbol{B}}{Dt} - \mathsf{W}\boldsymbol{B}.$$

Note that a sum of objective derivatives will also be objective and the Jaumann rate is a linear combination of the upper- and lower- convected derivatives

$$\overset{\circ}{\boldsymbol{B}} = \frac{1}{2}\left(\boldsymbol{B}^{\nabla} + \boldsymbol{B}^{\Delta}\right).$$

Tensors

Objective rates for tensors of higher order can be constructed from the same ideas. If we consider the material derivative of a convected second order tensor

$$\frac{D\mathsf{A}}{Dt} = \frac{D}{Dt}\left(A^{ij}\boldsymbol{G}_i \otimes \boldsymbol{G}_j\right) = \frac{\partial A^{ij}}{\partial t}\boldsymbol{G}_i \otimes \boldsymbol{G}_j + A^{ij}\left[\frac{D\boldsymbol{G}_i}{Dt} \otimes \boldsymbol{G}_j + \boldsymbol{G}_i \otimes \frac{D\boldsymbol{G}_j}{Dt}\right].$$

[6] We know that $\mathsf{F}^* = \mathsf{R}^*\mathsf{U}^* = \mathsf{QRU}$ and the polar decomposition is unique. QR is the product of two orthogonal matrices so it is orthogonal and by uniqueness of the polar decomposition $\mathsf{R}^* = \mathsf{QR}$.

$$= \frac{\partial A^{ij}}{\partial t} \boldsymbol{G}_i \otimes \boldsymbol{G}_j + A^{ij} \left[V^l||_i \boldsymbol{G}_l \otimes \boldsymbol{G}_j + \boldsymbol{G}_i \otimes V^l||_j \boldsymbol{G}_l \right] = \left[\frac{\partial A^{ij}}{\partial t} + A^{lj} V^i||_l + A^{il} V^j||_l \right] \boldsymbol{G}_i \otimes \boldsymbol{G}_j,$$

we can define the upper convected derivative

$$A^{\nabla \bar{i}\bar{j}} = \frac{DA^{\bar{i}\bar{j}}}{Dt} - A^{\bar{l}\bar{j}} V^{\bar{i}}||_{\bar{l}} - A^{\bar{i}\bar{l}} V^{\bar{j}}||_{\bar{l}}, \quad \text{or} \quad \mathsf{A}^{\nabla} = \frac{D\mathsf{A}}{Dt} - \mathsf{LA} - \mathsf{AL}^T;$$

and the lower convected derivative is found to be

$$A^{\Delta}{}_{\bar{i}\bar{j}} = \frac{DA_{\bar{i}\bar{j}}}{Dt} + A_{\bar{l}\bar{j}} V^{\bar{l}}||_{\bar{i}} + A_{\bar{i}\bar{l}} V^{\bar{l}}||_{\bar{j}}, \quad \text{or} \quad \mathsf{A}^{\Delta} = \frac{D\mathsf{A}}{Dt} + \mathsf{L}^T\mathsf{A} + \mathsf{AL}.$$

The Jaumann rate for a second-order tensor is formed from the appropriate linear combination of the upper and lower convected derivatives.

$$\mathring{\mathsf{A}} = \frac{1}{2}\left(\mathsf{A}^{\nabla} + \mathsf{A}^{\Delta}\right) = \frac{D\mathsf{A}}{Dt} + \frac{1}{2}\left(\mathsf{L}^T - L\right)\mathsf{A} + \mathsf{A}\frac{1}{2}\left(\mathsf{L} - \mathsf{L}^T\right) = \frac{D\mathsf{A}}{Dt} - \mathsf{WA} + \mathsf{AW}.$$

5.3 Example: An Ideal Gas

For a simple example of constitutive modelling, we consider an ideal gas, a gas in which the constituent molecules do not interact. Thus there can be no heat, energy or momentum transfer between molecules. In other words, an ideal gas has no dissipation, no deviatoric[7] stress and no heat flux. The behaviour of an ideal gas is unaffected by any deformations other than a change in material volume, J from equation (2.41b), which is equivalent to a change in density via conservation of mass $\rho = \rho_0/J$. Lecture 16

Thus, in our constitutive model, we expect the internal energy, stress and entropy to depend only on the density and temperature.

$$\Phi(\rho, \Theta), \quad \mathsf{T}(\rho, \Theta), \quad \eta(\rho, \Theta).$$

We should remember, of course, that all these quantities are functions of space and time, *e.g.* $\Phi(\boldsymbol{R}, t) = \Phi(\rho(\boldsymbol{R}, t), \Theta(\boldsymbol{R}, t))$. Under a change in Eulerian observer given by $\boldsymbol{R}^* = \mathsf{Q}(t)\boldsymbol{R}$, these quantities become

$$\Phi^*(\rho^*, \Theta^*) = \Phi(\rho, \Theta), \quad \mathsf{T}^*(\rho^*, \Theta^*) = \mathsf{QT}(\rho, \Theta)\mathsf{Q}^T, \quad \eta^*(\rho^*, \Theta^*) = \eta(\rho, \Theta).$$

The temperature and density are scalar fields and remain invariant under observer transform, so

$$\Phi^*(\rho, \Theta) = \Phi(\rho, \Theta), \quad \mathsf{T}^*(\rho, \Theta) = \mathsf{QT}(\rho, \Theta)\mathsf{Q}^T, \quad \eta^*(\rho, \Theta) = \eta(\rho, \Theta). \tag{5.4}$$

In order for the constitutive relations to be objective they must not change under observer transformation and because they are functions only of scalar variables, $\Phi^* = \Phi$, $\mathsf{T}^* = \mathsf{T}$ and $\eta^* = \eta$. The internal energy and entropy are also scalar fields, so these constraints are trivially satisfied from equation (5.4). The condition for the Cauchy stress is

$$\mathsf{T} = \mathsf{QTQ}^T,$$

[7]The deviatoric stress is the difference, or deviation, between the stress and the stress that would result if the only contribution is from a pressure load

$$\widetilde{\mathsf{T}} = \mathsf{T} - \frac{1}{3}\text{trace}(\mathsf{T})\,\mathsf{I}.$$

for all orthogonal matrices Q. Thus the stress tensor must be isotropic, *i.e.* it has no preferred direction, and so it must be a multiple of the identity matrix

$$\mathsf{T} = -P(\rho, \Theta)\mathsf{I}, \tag{5.5}$$

where P is called the thermodynamic pressure.

From the Clausius–Duhem inequality, using equation (4.27) in equation (4.25), we have the thermodynamic constraint

$$\rho\Theta\dot{\eta} - \rho\dot{\Phi} + \mathsf{T} : \mathsf{D} - \frac{1}{\Theta}\boldsymbol{Q}\boldsymbol{\cdot}\boldsymbol{\nabla}_{\boldsymbol{R}}\Theta \geq 0,$$

An ideal gas cannot support a heat flux, so

$$\rho\Theta\dot{\eta} - \rho\dot{\Phi} + \mathsf{T} : \mathsf{D} \geq 0. \tag{5.6}$$

We use the chain rule to expand all derivatives in terms of the variables ρ and Θ,

$$\dot{\eta} = \frac{\partial \eta}{\partial \rho}\dot{\rho} + \frac{\partial \eta}{\partial \Theta}\dot{\Theta}, \quad \dot{\Phi} = \frac{\partial \Phi}{\partial \rho}\dot{\rho} + \frac{\partial \Phi}{\partial \Theta}\dot{\Theta},$$

and use conservation of mass in Eulerian form (4.4) to write

$$\dot{\rho} = -\rho\boldsymbol{\nabla}_{\boldsymbol{R}}\boldsymbol{\cdot}\boldsymbol{V} = -\rho\,\mathrm{trace}(\mathsf{D}) = -\rho\mathsf{D} : \mathsf{I}. \tag{5.7}$$

Hence, equation (5.6) becomes

$$\rho\Theta\left(-\frac{\partial \eta}{\partial \rho}\rho\mathsf{D} : \mathsf{I} + \frac{\partial \eta}{\partial \Theta}\dot{\Theta}\right) - \rho\left(-\frac{\partial \Phi}{\partial \rho}\rho\mathsf{D} : \mathsf{I} + \frac{\partial \Phi}{\partial \Theta}\dot{\Theta}\right) + \mathsf{T} : \mathsf{D} \geq 0,$$

and after using equation (5.5)

$$\Rightarrow \quad \left[-P - \rho^2\Theta\frac{\partial \eta}{\partial \rho} + \rho^2\frac{\partial \Phi}{\partial \rho}\right]\mathsf{I} : \mathsf{D} + \left[\rho\Theta\frac{\partial \eta}{\partial \Theta} - \rho\frac{\partial \Phi}{\partial \Theta}\right]\dot{\Theta} \geq 0. \tag{5.8}$$

We can vary the relative volume change (or divergence of velocity) independently of the temperature and the inequality must be valid for all possible variations. In particular, for an isothermal process ($\dot{\Theta} = 0$), the inequality (5.8) must be satisfied for both positive and negative values of $\mathsf{I} : \mathsf{D}$, which means that

$$P = \rho^2\frac{\partial \Phi}{\partial \rho} - \rho^2\Theta\frac{\partial \eta}{\partial \rho}, \tag{5.9a}$$

because none of the quantities in equation (5.9a) depend on $\mathsf{I} : \mathsf{D}$. Similarly, for an isochoric ($\mathsf{I} : \mathsf{D} = 0$) processes, the inequality (5.8) must be satisfied for positive and negative values of $\dot{\Theta}$, so

$$\frac{\partial \Phi}{\partial \Theta} = \Theta\frac{\partial \eta}{\partial \Theta}. \tag{5.9b}$$

Equations (5.9a,b) are constraints that must be satisfied by our constitutive equations and they relate the pressure, entropy and internal energy.

We still need so-called equations of state that relate the pressure and energy to the temperature and density. A molecular model of a monatomic ideal gas considers N molecules (atoms), each with mass m and velocity $\boldsymbol{V}^{(i)}$. The atoms do not influence each other and can even pass through each other without any effect. The gas has only kinetic energy and the energy density is therefore given by

$$\Phi = \frac{\sum_i \frac{1}{2} m \boldsymbol{V}^{(i)} \cdot \boldsymbol{V}^{(i)}}{\sum_i m} = \frac{1}{2}\frac{1}{N}\sum_i \boldsymbol{V}^{(i)} \cdot \boldsymbol{V}^{(i)} \equiv \frac{1}{2}\langle \boldsymbol{V} \cdot \boldsymbol{V} \rangle, \tag{5.10}$$

where the angle brackets represent the average over all atoms. The corresponding temperature is given by

$$\Theta = \frac{m\langle \boldsymbol{V} \cdot \boldsymbol{V} \rangle}{3k_B}, \tag{5.11}$$

where k_B is the Boltzmann constant[8]. Using (5.11) to replace the term $\langle \boldsymbol{V} \cdot \boldsymbol{V} \rangle$ in equation (5.10), we obtain

$$\Phi = \frac{3k_B}{2m}\Theta = c_v \Theta, \tag{5.12}$$

where $c_v > 0$ is a constant called the specific heat of the gas at constant volume and Φ is therefore a linear function of Θ.

If we now imagine that the gas is in a piston that can move to change the volume then the normal force exerted on the piston head by a single atom is given by the negative[9] of the rate of change in momentum of the atom during its collision with the piston, $f_n^{(i)} = -\dot{p}^{(i)}$. If we assume perfectly elastic collisions then the change in momentum in a collision is simply $\Delta p^{(i)} = -2mV_n^{(i)}$, where $V_n^{(i)} > 0$ is the velocity component normal to the piston measured in the direction of the normal into to the piston. The time between collisions of a particular atom with the piston is given by $\Delta t^{(i)} = 2L/V_n^{(i)}$, where L is the length of the piston chamber. Thus, assuming that the piston is small enough (*i.e.* the time $\Delta t^{(i)}$ is very small) that the rate of change of momentum is well approximated by $\Delta p^{(i)}/\Delta t^{(i)}$, the average force exerted on the piston by all the atoms is given by

$$\langle f_n \rangle = \frac{1}{N}\sum_i -\frac{-2mV_n^{(i)}}{2L/V_n^{(i)}} = \frac{m}{L}\langle V_n^2 \rangle.$$

There is no preferred direction in the atom's motion, so we can write[10]

$$\langle \boldsymbol{V} \cdot \boldsymbol{V} \rangle = 3\langle V_n^2 \rangle.$$

Hence,

$$\langle f_n \rangle = \frac{m}{3L}\langle \boldsymbol{V} \cdot \boldsymbol{V} \rangle = \frac{k_B \Theta}{L},$$

from equation (5.11), and the pressure exerted on the piston is the total force per unit cross-sectional area

$$P = \frac{N\langle f_n \rangle}{A} = \frac{N k_B \Theta}{V},$$

[8]This result follows from the equipartition theorem of statistical physics that we don't have time to get into.

[9]This is negative because it is equal and opposite to the force exerted by the piston on the atom that causes the change in momentum.

[10]This result is obtained by considering a Cartesian coordinate system with one direction, say X_3, aligned with the normal direction to the piston, then

$$\langle \boldsymbol{V} \cdot \boldsymbol{V} \rangle = \langle V_I V_I \rangle.$$

If there is no preferred direction then

$$\langle V_1 V_1 \rangle = \langle V_2 V_2 \rangle = \langle V_3 V_3 \rangle,$$

and hence the result.

where A is the are of the piston and $V = LA$ is the volume of the piston chamber. In other words,

$$P = \rho R \Theta, \tag{5.13}$$

where $R = k_B/m > 0$ is the specific gas constant for the ideal gas in question. The equation (5.13) is of course the ideal gas law that was originally deduced from experiments.

Having deduced the constitutive equations (5.12) and (5.13) we can use the thermodynamic constraints (5.9a,b) to determine an expression for the entropy. Substituting (5.12) and (5.13) into (5.9a,b) we obtain

$$\rho R \Theta = -\rho^2 \Theta \frac{\partial \eta}{\partial \rho} \quad \text{and} \quad c_v = \Theta \frac{\partial \eta}{\partial \Theta},$$
$$\Rightarrow \quad \frac{\partial \eta}{\partial \rho} = -\frac{R}{\rho} \quad \text{and} \quad \frac{\partial \eta}{\partial \Theta} = \frac{c_v}{\Theta},$$

and integrating gives

$$\eta(\rho, \Theta) = c_v \log \Theta - R \log \rho + \eta_*, \tag{5.14}$$

where η_* is a reference entropy value.

We can now use our constitutive relations to determine the governing equations of gas dynamics. Conservation of mass is unaffected by the constitutive relations, but we must incorporate our expression for the stress into the linear momentum and energy equations. The balance of angular momentum is ensured by the symmetry of the stress tensor.

The governing equations of gas dynamics are therefore

$$\frac{D\rho}{Dt} + \rho \boldsymbol{\nabla}_{\boldsymbol{R}} \boldsymbol{\cdot} \boldsymbol{V} = 0,$$
$$\rho \frac{D\boldsymbol{V}}{Dt} + \boldsymbol{\nabla}_{\boldsymbol{R}} \boldsymbol{\cdot} (P\, \mathsf{I}) - \rho \boldsymbol{F} = \boldsymbol{0},$$
$$\rho \frac{D\Phi}{Dt} + P\, \mathsf{I} : \mathsf{D} - \rho B = 0.$$

We already know that $\mathsf{I} : \mathsf{D} = \boldsymbol{\nabla}_{\boldsymbol{R}} \boldsymbol{\cdot} \boldsymbol{V}$, and

$$[\boldsymbol{\nabla}_{\boldsymbol{R}} \boldsymbol{\cdot} (P\, \mathsf{I})]_K = (P\, \delta_{KJ})_{,J} = P_{,J}\, \delta_{KJ} = P_{,K} = [\boldsymbol{\nabla}_{\boldsymbol{R}}\, P]_K \,.$$

Thus, our final expression for the governing equations is

$$\frac{D\rho}{Dt} + \rho \boldsymbol{\nabla}_{\boldsymbol{R}} \boldsymbol{\cdot} \boldsymbol{V} = 0, \tag{5.15a}$$
$$\rho \frac{D\boldsymbol{V}}{Dt} + \boldsymbol{\nabla}_{\boldsymbol{R}}\, P - \rho \boldsymbol{F} = \boldsymbol{0}, \tag{5.15b}$$
$$\rho \frac{D\Phi}{Dt} + P\, \boldsymbol{\nabla}_{\boldsymbol{R}} \boldsymbol{\cdot} \boldsymbol{V} - \rho B = 0. \tag{5.15c}$$

Note that these equations are valid for any equations of state (not just an ideal gas) provided that $\mathsf{T} = -P(\rho, \Theta)\, \mathsf{I}$ and the thermodynamic constraints are satisfied.